Detection Techniques for Mobile Molecular Communication

Synopsis of the Thesis to be submitted in Partial Fulfillment of the Requirements for the Award of the Degree of

by

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Declaration by the Student

Date: 13/7/21

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This is to certify that the thesis entitled **Detection Techniques for Mobile Molecular Communication**, submitted by **Amit Kumar Shrivastava** to International Institute of Information Technology, Naya Raipur, is a record of bona fide research work under our supervision and we consider it worthy of consideration for the Synopsis of the Thesis to be submitted in partial fulfillment of the requirements for the award of the degree of Doctor of Philosophy of the Institute.

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Abstract

Molecular communication (MC) has been proposed as a means of coordination in nanonetworks, where information is exchanged between devices via molecules emitted and absorbed by each device. MC is used in health applications like Targeted Drug Delivery (TDD), where the nanomachines may be mobile and need to communicate with one another. Thus, investigation in mobile molecular communication (MMC) is essential in TDD application. However, communication in the MMC environment is challenging due to the mobile nature of nanomachines, especially for robust transmission and detection mechanisms. During communication, transmitted molecules undergo random movement according to the Brownian motion. Further, based on Einstein's theory of diffusion, the channel impulse response (CIR) varies with time and distance between the nanomachines. This variation affects the concentration of the molecules at the receiver, and so the detection techniques.

At first, the thesis proposes two non-coherent differential detection schemes, concentration difference-based detector (CDD) and manchester coded transmission with differential detection (MCD) for MMC. The detection threshold is selected using the maximum a posteriori probability (MAP) rule. The proposed CDD and MCD techniques do not need an adaptive threshold to detect the bit. The performance of these detectors is compared with other existing detection techniques single sample detector (SSD) and slope-based detector (SBD). Results reveal that CDD and MCD achieve a better bit error rate (BER) performance than SSD and SBD at 3 dB and 6 dB less signal-to-noise ratio (SNR), respectively. Moreover, the proposed CDD and MCD techniques perform better in different bit-sequence lengths, various initial distances, and different bit duration than other existing techniques. Detection is also affected by inter-symbol interference (ISI). To mitigate ISI, two coherent detection schemes, differential amplitude detection (DAD) and differential energy detection (DED), are proposed that utilizes the dynamic distance between the nanomachines for signal reconstruction. The detection is performed using the MAP rule, and the threshold is adjusted with the dynamic distance. Thus the effect of time-varying distance is taken into account by varying the detection threshold. Further, the proposed detection schemes, DED and DED, perform well for the channel having coherence time on the order of two-bit durations. The proposed DAD and DED detectors show better bit-error-rate (BER) performance than the concentration-based adaptive threshold detector (CATD). Both DAD and DED achieve a BER of 10^{-4} with BER of 0.1862 for CATD for coherence time of two-bit durations. Furthermore, the ~~p~~performances of the detection schemes are validated using particle-based simulation. For particle-based simulation, reactive receivers with circular receptors are considered, and simulations are performed with and without considering receptor occupancy. The detector finds two-time instants in the filtered signal to maximize the absolute concentration difference within the same bit duration. Subsequently, the concentration difference is used as the decision metric. Further, the BER of the proposed detection schemes is calculated using the analytical signal and validated using the particle-based signal. Simulation results show a good agreement between the BER obtained using the analytical signal and the particle-based signal. The performance analysis is then extended in light of the neural network (NN). In this endeavor, an NN-based detection is proposed for MMC. Three different techniques based on the filtered signal, slope values of the filtered signal, and concentration difference values of the filtered signal within a bit interval have been used for supervised training. The trained NN is used for detecting the unknown bits for time-varying parameters, such as the distance between transmitter (Tx) and receiver (Rx), noise, and the number of released molecules by the Tx. These algorithms train the NN faster compared to the first-order algorithms used in the existing works and the trained NN can perform well in a time-varying MMC environment. Overall, the thesis presents different detection schemes with better BER performances with respect to various parameters thus leading to a fundamental contribution for the future study of molecular communications and analysis.

Keywords: Mobile Molecular Communication, Detection Techniques, BER performance, Particle-based Simulation, Neural-Network, Targeted Drug Delivery.

1. Introduction

Molecular communication (MC) has been proposed as a means of coordination in nanonetworks, where information is exchanged between devices via molecules emitted and absorbed by each device. In MC, natural and artificial nanomachines communicate by transmitting and receiving molecules. Such a mechanism is found in biology, e.g., bacteria use this to sense their local population, known as quorum sensing [1]. Applications of MC are found in different fields, including medical [2], control and detection of chemical reactions, computational biology, biology, environmental management, and preservation and communication among nanorobots.

The main driving force for engineering MC is the medical field with applications in lab-on-a-chip devices, cell-on-chips devices, point of care diagnostic chips, and targeted drug delivery (TDD). In an MC system, nanomachines are the basic elements whose size can vary from nanometers to few micrometers [3]. These nanomachines can carry the drugs, which provide therapeutic actions in the human body during sickness. These drugs must act on cells since the sickness is due to the disorder in cells.

Fig. 1 shows that how a typical TDD can be accomplished using MC. As an example, when a transmitter nanomachine sends some commands to the receiver nanomachine by using signaling molecules, the commands can be sent in the form of bits:

- [0 0] - Start releasing drug molecules.
- [0 1] - Increase the number of drug molecules.
- [1 0] - Decrease the number of drug molecules.
- [1 1] - Stop delivering drug molecules.

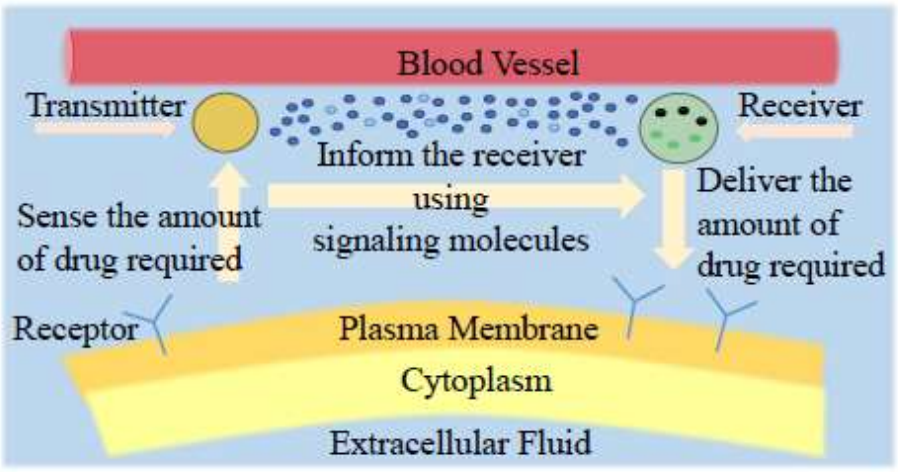

Fig. 1 Transmitter nanomachine (controller nanomachine) first senses the number of drug molecules required to be delivered inside the ECF. It can then send appropriate commands to the receiver nanomachine so that the receiver nanomachine (carrying drug molecules) can deliver the drug in the proper dose.

The receiver is an artificial nanomachine [4] that can release drug molecules based on the signaling molecules received from the transmitter nanomachines. Thus the appropriate transmission and detection are necessary. The complexity increases when nanomachines are mobile. Communication in the mobile molecular communication (MMC) environment is challenging due to the mobile nature of nanomachines, especially for robust transmission and detection mechanisms. During communication, transmitted molecules undergo random movement according to the Brownian motion. Also, the transmitter and the receiver are mobile in MMC. Due to mobility, the number of received molecules changes with the dynamic

distance between the transmitter and the receiver. An increase in distance causes fewer molecules to be received, thus reducing the SNR thereby increasing the BER. Hence, robust detection schemes for MMC are required.

In literature, a single sample detection scheme for MMC has been proposed in [5]. However, it does not perform well for increased mobility scenarios as it considers a fixed threshold for detection. The mobility can be increased due to enhance in the diffusion coefficient of the transmitter, the receiver, and the signaling molecules. Subsequently, detection in MMC based on local convexity of the received signal has been proposed in [6], [7]. Further, detection for MMC based on energy difference of the signals in consecutive bit intervals has been proposed in [8], where positive difference for bit-1 and negative difference for bit-0 was shown. MMC between a static transmitter and a mobile receiver is considered in [9], where the authors propose to reconstruct the channel impulse response (CIR) in each symbol interval using the time-varying transmitter-receiver distance estimated based on the peak value of the sampled concentration. Two adaptive schemes, i.e., concentration-based adaptive threshold detection and peak-time-based adaptive detection, are developed based on the reconstructed CIR. These techniques work well for the large coherence time of the channel, and robust detection schemes that perform well for low coherence time are also required in MMC. Further, in [10], different mobility cases, including mobile transmitter and receiver, mobile transmitter and fixed receiver, and mobile receiver and fixed transmitter, are considered to develop a stochastic channel model for diffusive mobile MC systems. The authors derive analytical expressions for the mean, pdf, and autocorrelation function (ACF) of the time-varying CIR through an approximation of the CIR with a log-normal distribution. Based on this approximation, a simple model for outdated channel state information (CSI) is derived. The detection performance of a single sample threshold detector relying on the outdated CSI is evaluated. In [11], the receiver estimates the initial distance between it and the transmitter. The estimated initial distance can be used to reconstruct the statistical characteristics of CIR, setting the detection threshold for all the bit intervals in advance. To achieve this goal, a novel two-step scheme based on maximum likelihood (ML) is proposed to estimate the initial distance. In the first step, the transmitter releases some molecules as a pilot signal before the information bits transmission. Then the receiver estimates releasing distance by observations of the received signal. In the second step, the estimated value obtained in the previous step is used to estimate the initial distance by ML estimation.

Noise due to other similar transmitters/counting noise and inter-symbol interference (ISI) often occur during this communication. ISI is due to the influence of received molecules in the previous symbol durations [7]. The receiver nanomachine will receive commands in the form of a bit sequence. Due to ISI, if command [0 1] is interpreted as [1 1], then instead of increasing the number of therapeutic molecules, the delivery of therapeutic molecules will be stopped, and the task of TDD will not be accomplished properly. Thus detection at the receiver and ISI mitigation [9] are important tasks at the receiver. Further, if the transmitter and the receiver are static, then the detection at the receiver is simple. However, if the transmitter and the receiver are mobile, then detection and ISI mitigation becomes challenging.

Further, the performance of the detection schemes needs validation through experiments or particle-based simulation. Particle-based simulation is an effective method to model the Brownian motion [12] of the transmitter, the receiver, and the signaling molecules and verify the performance of detection schemes. The work in [4] considers an advanced receiver model that determines the optimal release rate of molecules by identifying the causes of congestion in MC. Also, [13] studies stochastic ligand-receptor binding by considering each receptor as an M/M/1/1 queue where mean service time is equivalent to mean trafficking time. In [12], the analytical CIR is derived considering spherical receptors on the receiver's surface. However, triangular receptors of equal area are used for simulation. Circular receptors have been used in both analytical and particle-based simulations. A practical experiment showing differences due to the

geometry of the receptors has been shown in [14]. Human mesenchymal stem cells (hMSCs) were cultured on the three micropatterned shapes (triangular, square, and circular) for 24 hours. The intensity of lipid raft markers (that affects signal transduction) was different for triangular and circular receptors. Therefore, it is important to consider the similar geometry of receptors for analysis and simulation.

Furthermore, if the channel model is not known or difficult to obtain, then neural network (NN)-based detection [15] without CSI can be a good alternative to the conventional detectors that require CSI. An NN detector based on gradient descent (GD) optimization with adaptive threshold detection is proposed in [16]. Adaptive threshold detection is performed to counter the intersymbol interference (ISI), and it does not take into account the time-varying distance between transmitter and receiver. In [17], the NN detector combines the Takagi-Sugeno (TS) fuzzy model in the first hidden layer and the polynomial approximation by Least Mean Squares (LMS) technique in the second hidden layer. A feed-forward NN detector using Levenberg-Marquardt (LM) optimization algorithm is proposed for static transmitter and receiver [18].

2. Challenges in MMC

Mobile MC requires robust transmission and detection mechanisms, which pose many challenges. One of the most important is the influence of the dynamic CIR. During communication, transmitted molecules undergo random movement according to the Brownian motion. Based on Einstein's theory of diffusion, the CIR of the channel varies with time and distance between the nanomachines. The concentration of molecules at the receiver first increases to a maximum value and decreases slowly, forming a long tail [9]. The prominent challenges are:

- Unlike static MC, the received signal depends on the distance between the mobile nanomachines in MMC. A fixed threshold in MMC can cause incorrect signal detection.
- The dynamic behavior of CIR can make a more significant impact on signal detection due to ISI. For detection and ISI mitigation in MMC, tracking of the dynamic distance between the nanomachines is required. Thus, the detection process needs to be adaptive, i.e., the detection threshold adjustment is essential based on the distance between the transmitter and the receiver nanomachines.
- Further, the CSI is challenging to obtain due to multiple parameter variations in MMC using conventional detectors. Thus, robust detection schemes that perform well for multiple parameter variations are required for MMC.
- Also, the performance validation of the detection schemes is required. Performance validation may be done using experiments or particle-based simulations.

3. Motivation and Objectives

Based on the above challenges, robust and low complexity detection schemes are required for MMC. Further, efficient detection schemes are needed to perform well in fast varying diffusive channels for ISI mitigation. These detection schemes should have better BER performance in the MMC channel and also perform well in a real-time environment. The performance evaluation also needs to evaluate in light of future evolving techniques without CSI. Hence, the following objectives have been defined in this thesis:

- To develop low complexity non-coherent detection technique for MMC.
- To design coherent detection schemes with ISI mitigation for MMC to improve the BER performance at reduced SNR.
- To estimate dynamic distance in each bit interval for accurate signal reconstruction.
- To validate the performance in particle-based simulation in MMC.

- To investigate the performance with the help of neural-network-based detection for MMC.

4. Contributions to the thesis

4.1 Low complexity non-coherent detection for mobile molecular communication [M3], [M6]:

- Two differential detection schemes, concentration difference-based detector (CDD) and manchester coded transmission with differential detection (MCD) for robust performance in MMC environment, are proposed for TDD application.
- The proposed CDD and MCD techniques do not need an adaptive threshold to detect the bits. The techniques are relatively less sensitive to ISI and perform better at a particular signal-to-noise ratio (SNR). The performance of these detectors is compared with other existing detection techniques single sample detector (SSD) and slope-based detector (SBD).
- The proposed CDD and MCD techniques perform better in different bit-sequence lengths, various initial distances, and different bit duration than other existing techniques.

4.2 Coherent detection for mobile molecular communication [M1] [M7], [M8]:

- Adaptive threshold detection and ISI mitigation (ATDI) is proposed that utilizes the dynamic distance between the nanomachines for signal reconstruction and ISI mitigation.
- Differential amplitude detection (DAD) and differential energy detection (DED) with ISI mitigation are proposed for better BER performance.
- The proposed detection schemes, DED and DED, perform well for the channel having coherence time on the order of two-bit durations. Both the detectors, DAD and DED, show better bit-error-rate (BER) performance than the concentration-based adaptive threshold detector (CATD). The performance of both the detectors degrades with a decrease in coherence time.

4.3 Validation of the performance with particle-based simulation for reactive receiver [M5]:

- The BER performance of the proposed detection schemes is validated by particle-based simulation for a reactive receiver, where the Brownian motion of nanomachines and the signaling molecules is simulated.
- For particle-based simulation, reactive receivers with circular receptors are considered, and simulations are performed with and without considering receptor occupancy.
- The performances of the proposed detection schemes are calculated using the analytical signal and validated using the particle-based signal. Simulation results show a good agreement between the BER obtained using the analytical signal and the particle-based signal.

4.4 Neural network-based detection for mobile molecular communication [M4], [M9], [M11], [M12]:

- A neural network (NN) detector is proposed that does not require CSI.
- A second-order algorithm, Broyden–Fletcher–Goldfarb–Shanno (BFGS), pseudo-second-order algorithms Levenberg-Marquardt (LM), and scaled conjugate gradient (SCG) are used for training the NN.
- These algorithms train the NN faster compared to the first-order algorithms used in the existing works.
- Three different techniques based on (a) only the filtered signal, (b) slope of the filtered signal, and (c) concentration difference of the filtered signal have been used in conjunction with the BFGS, LM, and SCG algorithms for training the NN.

5. Work done in the thesis

The thesis proposes various low complexity non-coherent detection schemes for MMC. In this section, the investigations reported in the thesis (as mentioned above) are presented in brief with introductions to the basic ideas and the result obtained from the respective studies.

5.1 Non-coherent detection

In MMC, a nano-transmitter and a nano-receiver are considered to be in Brownian motion in an extracellular fluid medium. Transmitter uses calcium molecules to communicate with the receiver. Concentration difference-based detector (CDD) and manchester coded transmission with differential detection (MCD) for robust performance in MMC environment are proposed for TDD application. Detection is performed using CDD at the receiver, which calculates the maximum absolute concentration difference of the received signal within the same bit interval to detect the bit. This improves the BER performance in MMC. The performance is further enhanced using MCD. In MCD, *bit*-1 is coded by the symbol [1 0], and *bit*-0 is coded by the symbol [0 1], and the difference between peaks of signals received in consecutive bit duration is taken to detect the bit. Simulation results prove that the MCD technique is 3 dB less sensitive to ISI than the CDD technique. The detection threshold is selected using the MAP rule. The performance of these detectors is compared with other existing detection techniques. Results reveal that BER performance of the CDD and MCD better by at least 3 dB and 6 dB, respectively. The proposed CDD and MCD techniques perform better in different bit-sequence lengths, various initial distances, and different bit duration than other existing techniques.

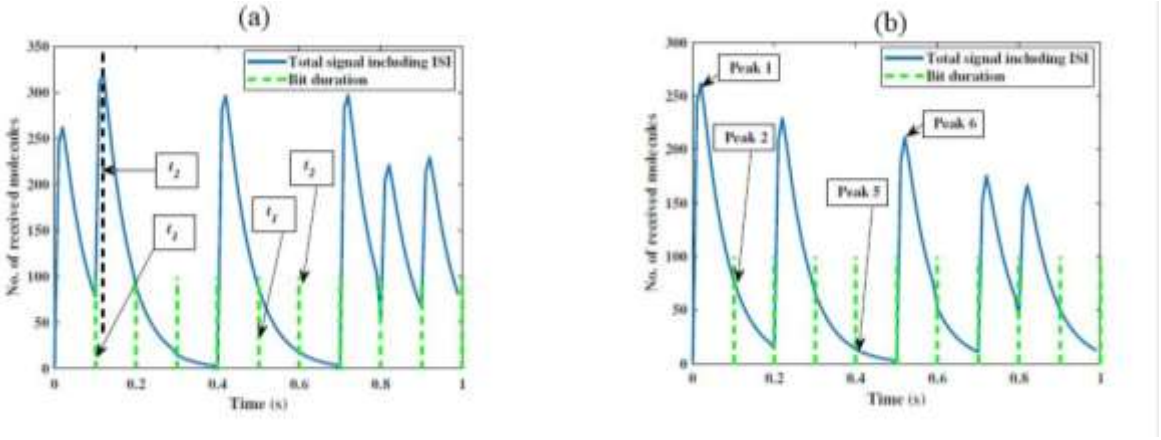

Fig. 2: The received signals for (a) CDD for transmitted sequence [1 1 0 0 1 0 0 1 1 1] and (b) MCD for transmitted sequence [1 1 0 0 1].

The received signal corresponding to CDD is shown in Fig. 2(a). CDD is used to detect whether the transmitted bit was a bit-0 or a bit-1. For detection, the difference between the concentration at two different time instants t_2 and t_1 within each symbol interval is calculated such that the absolute difference is maximized. The difference between these two-time instants t_2 and t_1 is then used as the decision metric. The received signal corresponding to the MCD technique is shown in Fig. 2(b). The differential detector calculates the difference between peaks of consecutive bits in a symbol. This difference is positive when symbol [1 0] is received, and the difference is negative when symbol [0 1] is received.

The impact of increasing bit sequence length on BER for the different detectors is shown in Fig. 3. At 60 dB SNR, BER values become large for all detectors because, during transmission of more amount of bits, the distance between the nanomachines may increase, and fewer molecules might reach the receiver.

This effect can be reduced by increasing the SNR to 80 dB. A high value of SNR is required in MMC relative to static MC. This is because the distance between nanomachines may increase, leading to insufficient signal power if less value of SNR is used. At different SNR values, CDD gives a better performance than SBD and SSD. Also, MCD outperforms other detectors.

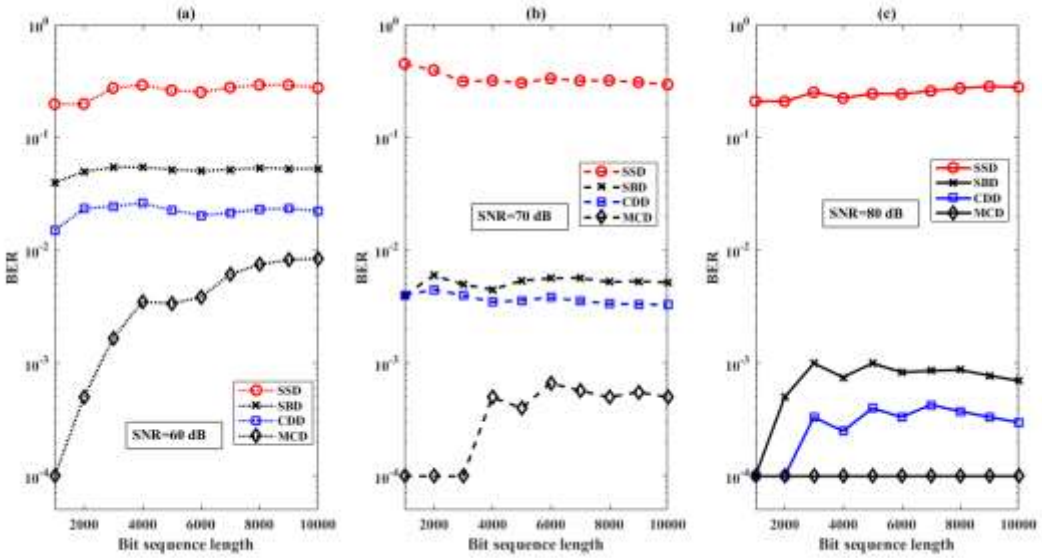

Fig. 3: Variation of BER with the bit-sequence length for different detection techniques at different SNR (a) 60 dB, (b) 70 dB, and (c) 80 dB.

5.2 Coherent detection

Due to the dynamic nature of nanomachines and diffusion channels, detection is challenging in MMC. In general, signal detection is performed on the number of received molecules with respect to a fixed threshold. However, in MMC number of received molecules varies in each bit interval, which makes detection very challenging if a fixed threshold is considered. In addition to this, the dynamic nature of nanomachines, communication channels impact ISI and make it time-varying. In this work, an adaptive threshold detection and ISI mitigation (ATDI) scheme is proposed for signal detection in MMC. The adaptive threshold selection depends on the parameters such as the dynamic distance between nanomachines, diffusion coefficient, etc. Detection using an adaptive threshold improves the detection performance and also mitigates the ISI manifold. The modified concentration shift keying (M-CSK) based modulation is used to release more amount of signaling molecules for bit-1 than bit-0. The received signal is reconstructed in each bit interval using the average distance variation in a bit interval. The reconstructed received signal is subtracted from the total received signal in subsequent bit duration. The detection threshold is calculated by applying the MAP rule to reconstructed signals for the bit-1 and the bit-0 of the previous bit interval. The performance of this detector is compared with an existing detection technique concentration-based adaptive threshold detector (CATD) [9].

The two detection techniques, namely differential amplitude detection (DAD) and differential energy detection (DED), are proposed for MMC, where transmit-receive (T-R) nanomachines are in Brownian motion. Spherical transmitter and reactive receiver are considered in the model. Manchester coded bits are transmitted using modified concentration-shift-keying. In the proposed detection mechanism, an adaptive threshold technique is used at the receiver to estimate the number of transmitted molecules

using the maximum a posteriori probability MAP rule. This helps to estimate the dynamic distance within a bit interval. The average dynamic distance in each bit interval helps to reconstruct the received signal. Subsequently, the ISI mitigation is performed by subtracting the reconstructed signals of previous bit intervals from the total received signal. Further, the detection is performed by taking the concentration difference between the peak amplitude of consecutive ISI mitigated signals in DAD. In DED, the difference in the energy of the signals is considered for detection. The performance of these detectors is compared with another existing detection technique. The proposed DAD & DED techniques perform better in terms of the coherence time of the channel, increasing diffusion coefficient, increasing initial distance, signal to noise ratio, and the number of samples. Particle-based simulation for the reactive receiver is also carried out to validate the results.

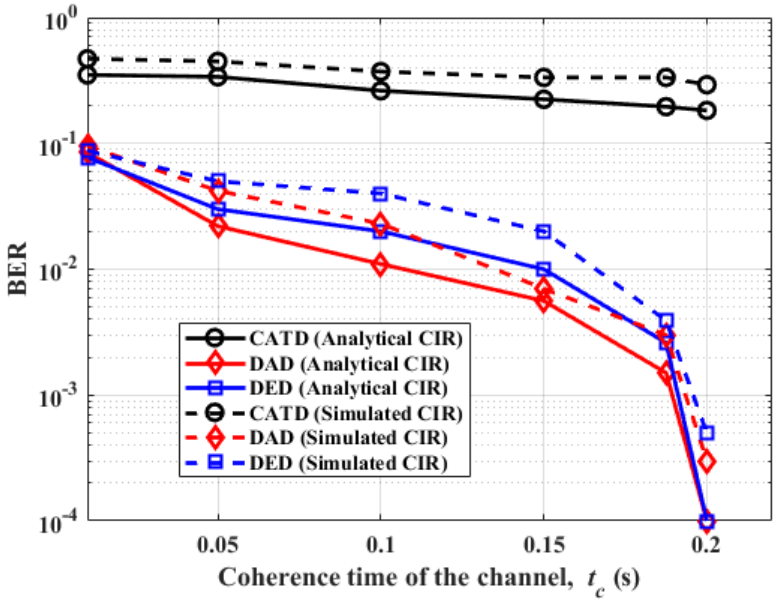

Fig. 4: BER versus coherence time of the channel.

For DAD and DED, the impact of coherence time on the BER is shown in Fig. 4. Values of coherence time t_c are shown in braces [0.01 s, 0.05 s, 0.1 s, 0.15 s, 0.1875 s, 0.2 s]. In terms of bit duration T, these values correspond to [T /10, T /2, 1.5 T, 1.875 T, 2T]. CATD [9] does not perform well, even when the coherence time is 2T. For detection in the current bit duration, it considers the threshold calculated during the bit duration in which the last bit-1 was transmitted. Channel can change considerably between the current bit duration and the bit duration in which the last bit-1 was transmitted. In this case, the threshold is not close to the correct value. Both DAD and DED achieve a BER of 10^{-4} for a coherence time of 2T, whereas CATD gives a BER of 0.1862. Also, DAD achieves a BER of 0.0015 for a coherence time of 1.875T, whereas DED gives a BER of 0.0026, and CATD has a BER of 0.1957 for the same coherence time. The performance of both the detectors degrades with a decrease in coherence time. The proposed detectors DAD and DED show a better BER performance than CATD.

5.3 Particle-based simulation

In this work, a particle-based simulation of two differential detectors for a reactive receiver in MMC is presented. The received signal is filtered and used for detection. On-off keying (OOK) is used as the modulation in both schemes. The detector in the first scheme finds two-time instants in the filtered signal

to maximize the absolute concentration difference within the same bit duration. Then the concentration difference is used as the decision metric. The second scheme uses Manchester coding at the transmitter where the bit-0 and bit-1 are represented as the symbol [0 1] and symbol [1 0], respectively. The difference between the peak values of filtered signals in successive bit durations is used as the decision metric. Correlation between the analytical signal and particle-based signal is also found. Further, the BER of the proposed detection schemes is calculated using the analytical signal and validated using the particle-based signal. Simulation results show a good agreement between the BER obtained using the analytical signal and the particle-based signal.

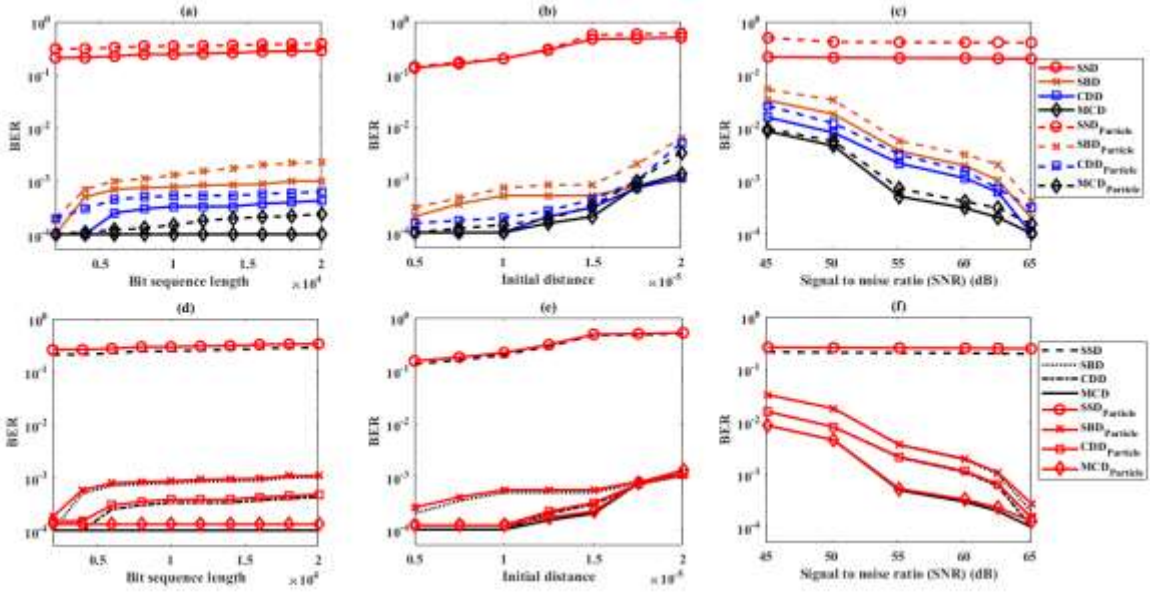

Fig. 5: (a)-(c) Effect of receptor occupancy is considered. (d)-(f) Effect of receptor occupancy is not considered in the particle-based simulation.

BER versus bit sequence length has been shown in Fig. 5(a). MCD gives the lowest BER, while CDD gives a BER slightly higher than the MCD. SSD has the worst BER performance because it uses a fixed threshold for detection. The SBD performs better than the SSD, while the SBD has high BER than the CDD and the MCD technique. The SBD uses the difference between adjacent samples as the decision metric. The positive difference may become negative and vice versa in noisy scenarios. The BER with increasing initial distance is shown in Fig. 5(b). As the distance increases, the signal power at the receiver reduces. Thus, the BER for all the detection schemes increases. Further, Fig. 5(c) shows the BER variation with the SNR. CDD and MCD achieve a BER of 10^{-3} at 61 dB and 53 dB, respectively. Also, the BER curves of the detectors using particle-based simulation are denoted as $SSD_{Particle}$, ,$SBD_{Particle}$, and $CDD_{Particle}$ and $MCD_{Particle}$. These are some deviations in the BER curves for analytical and simulation results due to the effect of receptor occupancy, as shown in Fig. 5(a)-(c). Further, suppose the effect of receptor occupancy is disabled in a particle-based simulation. In that case, the results of analytical and simulated BER are in good agreement, as shown in Fig. 5(d)-(f). Also, the bit rate for CDD is twice that of MCD.

Further, for a given distance between the transmitter and the receiver, the particle-based simulation is repeated to find the number of received molecules in each repetition. Since the motion of molecules is Brownian (random), the number of molecules received in each repetition is slightly different. The number of repetitions is termed iteration in this work, which affects the correlation coefficient. The correlation

coefficient varies between $0.97 - 0.99$ at the 10 μm distance between the transmitter and the receiver, which indicates a similarity of the analytical signal and the signal obtained using particle-based simulation within a distance of 10 μm. At a distance of 15 μm, the range of correlation coefficient drops to $0.91 - 0.96$. Thus, the BER obtained using the analytical signal and the particle-based signal does not match at a large distance ≈ 20 μm, as shown in Fig. 5(b). The amplitude of the particle-based signal is less than the amplitude of the analytical signal for a large number of transmitted molecules [12]. Thus at a large distance ≈ 20 μm, the SNR of the particle-based signal becomes less than the SNR obtained using the analytical signal. Hence, the BER obtained using the particle-based signal is larger than the BER obtained using the analytical signal. In the particle-based simulation, if a large number of signaling molecules are sent from the transmitter, more molecules arrive near the receiver. This effect increases the probability that some molecules collide with an occupied receptor. This leads to the difference between the analytical signal and the particle-based signal because the effect of receptor occupancy is not considered in the analytical model.

5.4 Neural Network Detector

In this work, a neural network (NN) detector for MMC has been proposed. The NN uses BFGS and LM algorithms for optimization. In the proposed work, the received signal is filtered, and three different techniques for supervised training and detection are used. The three different techniques are (a) the filtered signal, (b) slope values of the filtered signal, and (c) concentration difference values of the filtered signal within a bit interval. The trained NN is used for detecting the unknown bits for time-varying parameters such as the distance between transmitter and receiver, noise, and the number of released molecules by the transmitter.

BER with the signal-to-noise ratio (SNR) is shown for different parameters such as coherence time of the channel, diffusion coefficient of the transmitter, and the initial distance between the transmitter and the receiver. Simulation results show that the BFGS algorithm trains the NN faster compared to the LM algorithm, and the trained NN can perform well in a time-varying MMC environment.

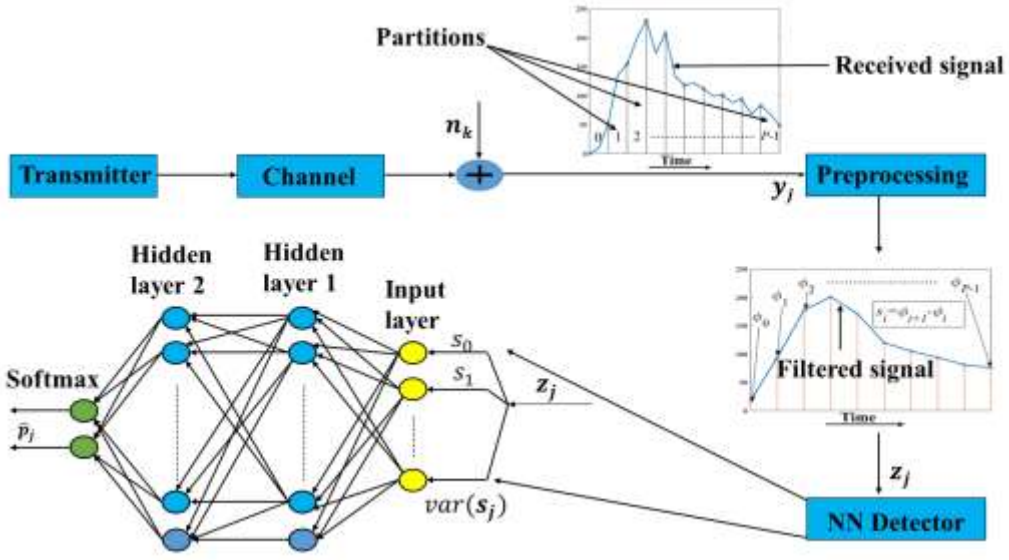

Fig. 6: Block diagram of the proposed NN-based detector for mobile MC.

The block diagram of the entire scheme is shown in Fig. 6. The number of transmitted molecules is *U* [40000 45000], and noise is *U* [0 5], where *U* [a b] denotes the uniform distribution over the range [a

b]. Channel is ECF, as shown in Fig. 1. The CIR varies due to i) the number of transmitted molecules, based on the availability of the molecules at the transmitter, ii) noise and iii) time-varying distance between the transmitter and the receiver. The receiver contains the NN detector having two hidden layers each of size 20. The final layer is the softmax layer. As shown in Fig. 6, filtering the received signal is done by partitioning the bit interval into equal subintervals and averaging the signal in each partition.

The NN is trained using 50000 bits. BFGS and LM algorithms have been used to minimize the loss function (cross-entropy) [15]. Fig. 7 shows the BER vs. SNR for different parameters. It can be observed from Fig. 7(i) that when $t_c \approx T$, the BER values are 4×10^{-4}, 3×10^{-4}, and 10^{-4} for NN detector trained with different the filtered signal, slope vector, and concentration difference vector respectively at 56 dB SNR. Results reveal a better performance of the NN detector than DBD primarily because of the use of fixed detection threshold [19], which is not suitable for MMC. Fig. 7 (i)-(iii) show that the BFGS algorithm achieves less BER if the concentration difference vector is used for training the NN. Further, the LM algorithm gives less BER if the filtered signal or slope vector are used for training, as shown in Fig. 7(iv)-(v).

Further, NN-based detection using a scaled conjugate gradient (SCG) algorithm for updating the weights of the NN is presented. Moreover, three different techniques are used in training and detection by the NN. These techniques correspond to i) filtered signal, ii) slope values of the filtered signal, and iii) concentration difference of the filtered signal in a bit interval. More specifically, a sequence of transmitted bit pattern and each of the above three techniques is used separately for training the NN. After training, the NN-based detector performs detection under a time-varying channel. The bit error rate BER performance of the proposed SCG algorithm for NN-based detector is also compared with a first-order algorithm Gradient Descent (GD) and a second-order algorithm BFGS for different coherence times of the channel. Simulation results demonstrate that the NN detector using SCG outperforms the BFGS if slope values are used for training the NN. Further, the SCG algorithm has a significant performance gain compared to the GD algorithm.

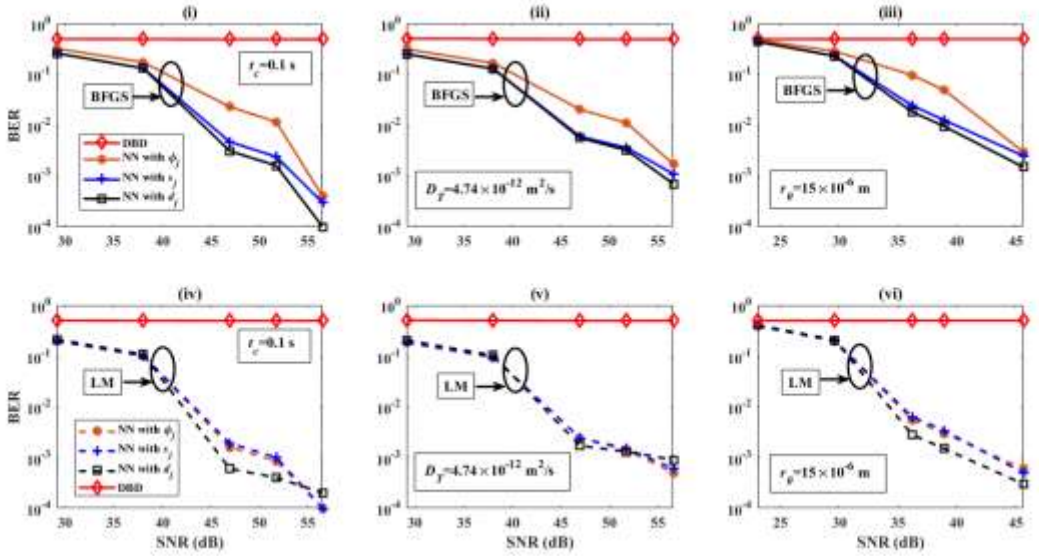

Fig. 7: BER versus SNR at different parameter values for (i)-(iii) BFGS optimizer (iv)-(vi) LM optimizer.

Fig. 8 shows the variation of BER with t_c for a fixed SNR of 56 dB. It can be seen that an increase in the value of t_c leads to a decrease in the BER because the channel variation becomes slow with an increase

in t_c. Further, one can observe in Fig. 8(a) that the SCG algorithm performs better than the GD and BFGS algorithms if slope values are used for training the NN detector. Moreover, Fig. 8(b) shows that if concentration difference is used, the BFGS algorithm outperforms GD and SCG. Furthermore, the performance of the SCG algorithm is comparable to the performance BFGS algorithm if the filtered signal is used, as seen in Fig. 8(c). Also, Table 1 shows the performance comparison of the proposed and existing NN detectors.

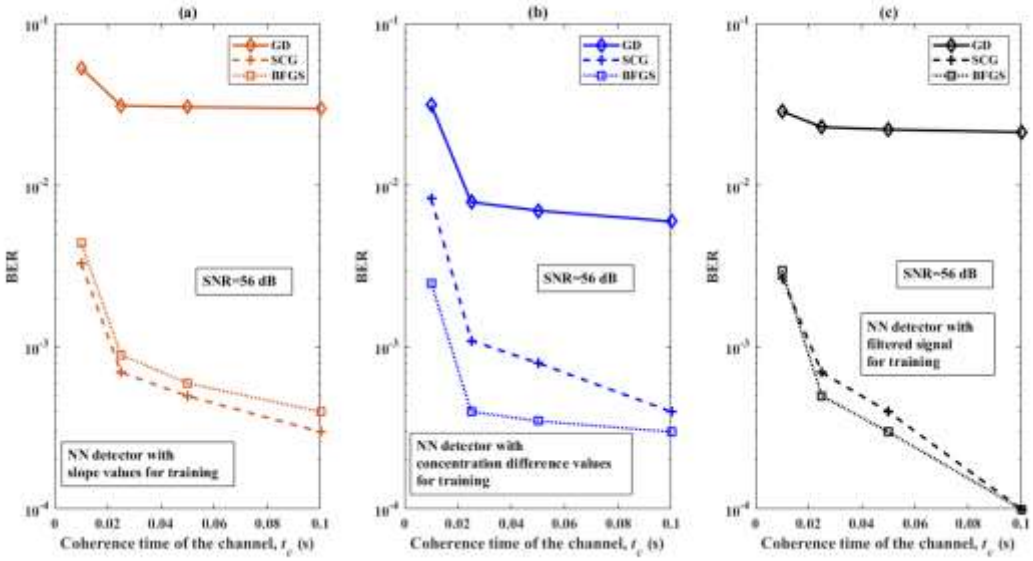

Fig. 8: BER versus t_c for (a) slope values (b) concentration difference values (c) filtered signal used in training the NN.

Table 1: Comparison of the proposed NN detector with existing NN detection schemes

Parameters	**NN detector with BFGS and LM**	**NN detector with SCG**	**Detectors in [15]**	**Detector in [18]**
Number of hidden layers	2	2	3	10
Nodes in each hidden layer	20	20	80	5
Optimizer	BFGS/LM	SCG	ADAM	LM
Order of optimizer	Second /Pseudo second (PS)	Between first and second	First	PS
Number of bits for training	50000	10000	500000 sequence of 100 bits	50000
Lowest BER achievable	10^{-4}	10^{-4}	3×10^{-5}	3×10^{-5}
Channel	Time-varying	Time-varying	Time-varying	Time-invariant

6. Conclusion and future work

The synopsis has introduced the topic of research undertaken in the present doctoral work and outlined the basic process of MMC with its application in TDD. In MMC, the requirement of robust detection techniques due to the degradation effects of noise and ISI was discussed. Next, the performance of a novel CDD technique for signal detection in an MMC scenario is evaluated. An MCD technique has

also been explored. Results reveal that CDD and MCD achieve a better BER performance than SSD and SBD at 3 dB and 6 dB less SNR, respectively, with other similar parameters. Then the performance evaluation of an adaptive detection technique in MMC is done. Performance of ATDI, DAD, and DED with ISI mitigation was are also discussed. Further, it has been shown that the error in the estimation of average distance in each bit interval lies within 5%-7%. The next work presents the particle-based simulation of CDD and MCD for a reactive receiver. The work has further been extended to develop NN-based detector for MMC. NN-based detectors do not require accurate CSI for signal detection and are useful for detection where channel models are difficult to obtain. Therefore, the multifaceted research outcome of this dissertation may help to advance molecular communication research.

The limitation of the present work and some comments on the future scope of research in this field are highlighted here. The proposed non-coherent detection schemes require high SNR values for better BER performance. Hence, improvement to the current scheme can be made in terms of reducing the SNR required for obtaining low BER. Further, in the coherent detection scheme, distance estimation, signal reconstruction, and ISI mitigation in every bit interval entails high complexity. So, reducing the complexity of the detection process can be one of the future works. Furthermore, experimental verification of the proposed detection schemes can be considered. In this work, perfect synchronization between the transmitter and the receiver is considered; however, the performance evaluation of these detectors considering synchronization error is still lacking. Also, in view of the current pandemic situation, end to end MC system model to track the propagation of coronavirus within the respiratory system can be considered as future work.

7. Organization of the thesis

The thesis organized as follows. **Chapter 1** provides a general introduction to molecular communication and an outline of the work reported in the thesis. The literature survey is presented in **Chapter 2**. **Chapter 3** presents the two non-coherent differential detection schemes, CCD & MCD for mobile MC that offers robust detection performance for TDD application. **Chapter 4** presents adaptive threshold detection and ISI mitigation (ATDI) that utilizes the dynamic distance between the nanomachines for signal reconstruction and ISI mitigation. Performance validation of the detection schemes using particle-based simulation is discussed in **Chapter 5**. **Chapter 6** proposes a neural network-based scheme for mobile molecular communication. Finally, **Chapter 7** presents the concluding remarks on the work along with the future scopes.

8. Publications from this thesis work

Indian Patent:

[M1] A. K. Shrivastava, D. Das, and R. Mahapatra, “Differential detectors with inter-symbol interference mitigation for mobile molecular communication” in process

Journals (Accepted)

[M2] A. K. Shrivastava, D. Das, N. Varshney, and R. Mahapatra, “Transmission and detection techniques for internet of bio-nano things applications with static and mobile molecular communication: A survey”, in *ITU - Journal on Future and Evolving Technologies*, 2021.

[M3] A. K. Shrivastava, D. Das, R. Mahapatra, and S. P. Mohanty, "dmole: A novel transreceiver for mobile molecular communication using robust differential detection techniques," *IEEE Transactions on NanoBioscience*, vol. 19, no. 4, pp. 609–621, 2020. **(I.F. 2.791)**

[M4] A. K. Shrivastava, D. Das, and R. Mahapatra "Performance evaluation of mobile molecular communication system using neural network detector*," IEEE Wireless Communications Letters* (Early Access), 2021, **DOI:**10.1109/LWC.2021.3079522. **(I.F. 4.66)**

[M5] A. K. Shrivastava, D. Das, and R. Mahapatra, "Particle-based simulation of the differential detectors for mobile molecular communication" in *IEEE Communications Letters*, (Early Access), 2021, **DOI:** 10.1109/LCOMM.2021.3093651. **(I.F. 3.419)**

Conferences (Accepted)

[M6] A. K. Shrivastava, D. Das, and R. Mahapatra, "Slope-based detection for mobile molecular communication based on Einstein's law of diffusion," in 2018 15th *IEEE India Council International Conference* (INDICON). IEEE, 2018, pp. 1–6.

[M7] A. K. Shrivastava, D. Das, and R. Mahapatra, "Adaptive threshold detection and ISI mitigation in mobile molecular communication," in 2020 *IEEE Wireless Communications and Networking Conference* (WCNC). IEEE, 2020, pp. 1–6.

Under review

Journal

[M8] A. K. Shrivastava, D. Das, and R. Mahapatra, "Particle-based simulation for detection and ISI mitigation in mobile molecular communication" in *IEEE Transactions on NanoBioscience*.

Conference

[M9] A. K. Shrivastava, D. Das, and R. Mahapatra, and N. Varshney, "Scaled conjugate gradient algorithms for neural network detector in mobile molecular communication" in *IEEE GLOBECOM* 2021.

Under preparation

[M10] A. K. Shrivastava, D. Das, and R. Mahapatra, "MIMO signal detection using neural network for mobile molecular communication," for *IEEE Transactions on Molecular, Biological and Multi-Scale Communications*.

[M11] A. K. Shrivastava, D. Das, and R. Mahapatra, "Machine learning algorithms to improve the performance of mobile molecular communication," for *IEEE Transactions on Communications*.

[M12] A. K. Shrivastava, D. Das, and R. Mahapatra, "Machine learning for mobile molecular communication: A survey" for *IEEE Communication Surveys and Tutorials*.

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